Identifying influential factors of solvents on heterogeneous enantioselective hydrogenation of methyl pyruvate through machine learning analysis

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Machine learning techniques are recently applied to the field of heterogeneous catalysis for predicting optimal compositions of catalysts and investigating key factors in the catalysis. In this study, we attempted to train the decision tree-based models and conducted feature importance analysis to investigate the solvent effect in heterogeneous enantioselective hydrogenation. The physicochemical properties of pure and mixed solvents were chosen as the input variables and the output variables for supervised learning were obtained from enantioselective hydrogenation of methyl pyruvate over 1 wt% Pt/Al_2O_3 catalyst. The key factors obtained from feature importance analysis were consistent with the domain knowledge in enantioselective hydrogenation of α-ketoesters. In addition, the results provided new information that has not been previously reported.